

Spin Qubits in Germanium Structures with Phononic Gap

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We propose qubits based on shallow donor electron spins in germanium structures with phononic gap. We consider a phononic crystal formed by periodic holes in Ge plate or a rigid cover / Ge layer / rigid substrate structure with gaps \sim a few GHz. The spin relaxation is suppressed dramatically, if the Zeeman frequency ω_Z is in the phononic gap, but an effective coupling between the spins of remote donors via exchange of virtual phonons remains essential. If ω_Z approaches to a gap edge in these structures, a long-range (limited by detuning of ω_Z) resonant exchange interaction takes place. We estimate that ratio of the exchange integral to the longitudinal relaxation rate exceeds 10^5 and lateral scale of resonant exchange ~ 0.1 mm. The exchange contribution can be verified under microwave pumping through oscillations of spin echo signal or through the differential absorption measurements. Efficient manipulation of spins due to the Rabi oscillations opens a new way for quantum information applications.

Introduction

Successful implementation of quantum information processing (QIP) requires not only invention of new quantum algorithms such as Shor algorithm, quantum error correction code or quantum adiabatic algorithm, but also further hardware development, i.e. realization of various qubit architectures - from trapped atoms to superconducting circuits.¹ A significant advantage of solid state systems, based on different types of quantum dots² or impurities in semiconductors,³⁻⁵ is a capability to fabricate, manipulate and read out qubits using semiconductor nanotechnology and conventional electronics. On the other hand, all reliable and efficient QIP schemes simultaneously require both long qubit decoherence times and controllable qubit manipulation, which poses a major challenge for practical implementation of these systems.⁶ Indeed, shallow donor spin qubits in semiconductors have a number of advantages related to these requirements due to tunable spin-lattice interaction and a possibility to control spin states without a charge-induced noise. At the same time, broadly investigated silicon-based donor qubits with large spin decoherence times suffer from limitations in controlling and manipulating spins due to weak spin-orbit interaction.⁶ Here we suggest a route for implementing new spin-qubit architectures based on donor spins embedded in specially crafted germanium structures (quasi-two-dimensional periodic phononic crystals or planar phonon waveguides) with large spin-orbit interaction of the Ge host and engineered phonon bandgaps to simultaneously suppress spin decoherence and enable strong spin-spin coupling between the qubits.

The large spin-orbit coupling inherent to shallow donors in bulk Ge enhances our ability to

manipulate the spin qubits but could be detrimental for their coherence. In fact, the spin relaxation time of donors in Ge bulk is three to four orders of magnitude shorter than that in Si. To cope with this problem we will utilize Ge-based artificial periodic structures, known as *phononic crystals* (PC).⁷ Similarly to the *photonic crystals*, that were invented to control the light,⁷ the phononic crystals of different dimensions can be used to control various types of acoustic waves, e.g. to filter and focus sound⁷ or even to create the earthquake proofing of buildings⁷. A proposed quasi-2D phononic crystal formed by a lattice of holes in a suspended Ge layer is shown in Fig 1-a. This structure is similar to recently manufactured Si-based PCs⁸ with ~ 100 nm period and thickness defining the phonon gap within GHz frequency domain. The phonon dispersion curves, shown in Fig. 1b, display pronounced gap in the frequency interval $13 \div 15$ GHz. If the Zeeman energy of the donor spin $\hbar\omega_Z$ is tuned inside the phonon gap the one-phonon spin-flip transitions will be forbidden due to energy conservation. As a result, the longitudinal relaxation rate, ν_1 , determined by very weak two-phonon processes, will be suppressed by five orders in magnitude compared to its bulk value. At the same time, the spin-lattice coupling will remain strong ($3 \div 4$ orders larger than in bulk silicon) and the spin-spin interaction via virtual one-phonon exchange processes will exceed ν_1 by many orders.

Similar behavior is possible if Ge layer is sandwiched between the rigid substrate and cover layers made from diamond, BN, or H-SiC (r/Ge/r-structure, see Fig. 2a). Penetration of vibrations from cover and substrate layers into Ge is weak because the reflection is effective due to the about 10 times differences⁹ between modules of elasticity in rigid materials and soft Ge. Thus, the spin-phonon interaction with bulk modes is ineffective and there is a gap for waveguide modes in Ge

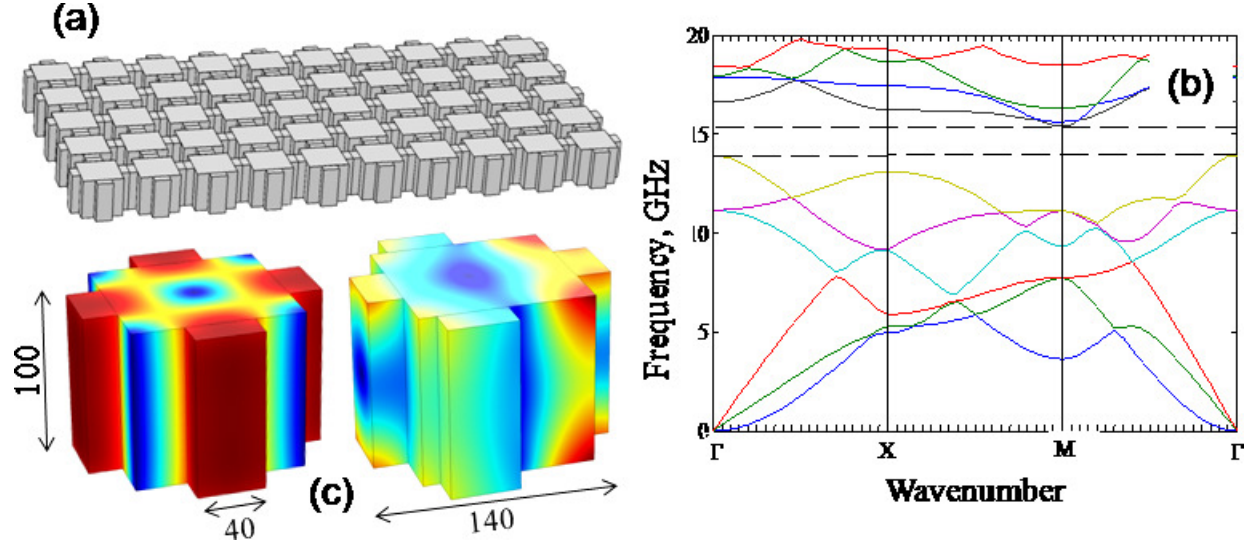


Figure 1: **Phononic crystal.** (a) Geometry of PC formed by square lattice of holes. (b) Dispersion laws along ΓX , ΓM , and XM directions with gap between 6th and 7th modes. (c) Distributions of displacements over the unit cells of symmetric (left) and nonsymmetric (right) PCs for 7th mode at M-point (colored from blue, correspondent zero to red); sizes?dimentions are in nm.

layer up to cut-off frequency in GHz range (Fig. 2b), so that ν_1 is suppressed but the exchange interaction via vibrations localized in Ge remains essential if $\hbar\omega_Z$ is in the phonon gap for waveguide modes. Once again, one obtains the donor spin system with an effective exchange interaction and a negligible ν_1 . If ω_Z is fine tuned to lie within a gap edge in these structures, both strength and lateral scale of a resonant exchange interaction (REI) enhance. Thus, a spin system with essential?strong (and long-range for REI-regime) interaction and suppressed relaxation (transverse rate ν_2 remains only) in PC or r/Ge/r-structure.

Both verification of the spin-Hamiltonian parameters and manipulation of spin coherence are possible under resonant microwave (mw) pumping of frequency $\omega \sim \omega_Z$. Under continuous mw pump, the exchange-renormalized ω_Z modifies a differential absorption shape in the linear response regime. An interplay between the Rabi oscillations frequency ω_R and the exchange con-

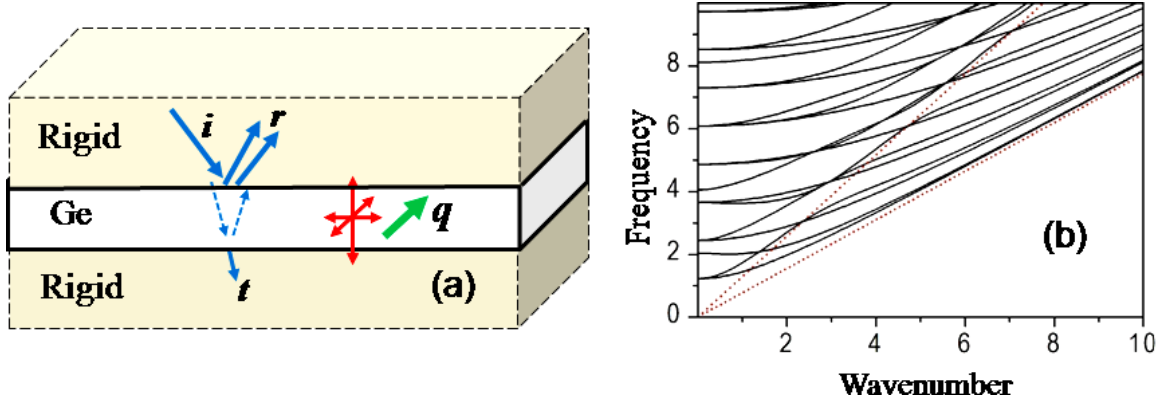


Figure 2: **Sandwiched Ge structure.** (a) r/Ge/r structure with Ge layer of width d ; incident (i -), reflected (r -), and transmitted (t -) waves and three waveguide modes (shear and coupled) with in-plane wave vector q are shown. (b) Dispersion laws (frequencies in $2\sqrt{c_l c_t}/d$ versus wavevector in $2/d$) with gap up to cut-off frequency $\pi c_t/d$.

tributions to Zeeman frequency ($\omega_{1,2} - \omega_Z$, see Fig. 3a) takes place for the nonlinear pumping case and it modifies a nonlinear differential absorption. If dephasing processes and long-range disorder are essential, a two-pulse spin echo measurements¹⁰ enable to extract the exchange renormalization of ω_Z . Fig. 3b shows the sequence $(\pi/4 - \tau - 3\pi/4 - \tau \rightarrow \text{echo signal})$ with different frequencies of free rotation during τ -delay intervals. As a result, an echo amplitude oscillates with τ , if $\omega_{1,2} \neq \omega_Z$. Beside of this, a multi-pulse spin echo scheme can be applied for manipulation of averaged spin orientation.

Summarizing the results obtained, we have demonstrated that a controllable manipulation of in quasi-free spin system in PC or r/Ge/r-structures is possible by the reasons:

- i/ strong suppression of relaxation-to-exchange ratio (in contrast to the bulk case¹³) opens a way for fault-tolerant operations;
- ii/ very sharp (at detunings $\delta_Z \leq 10^{-3}$ correspondent a weak variations of magnetic field) transformation from free spin system to large-scale REI-regime permits a remote control of qbits, with-

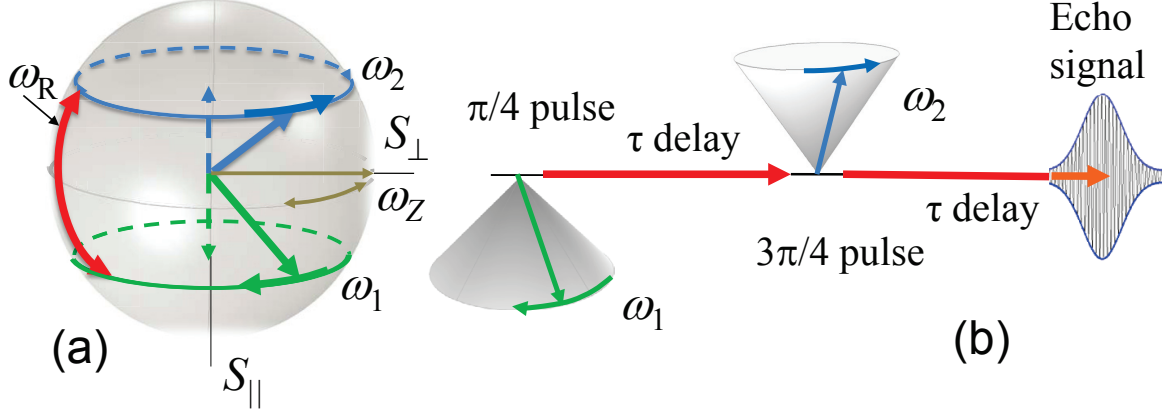


Figure 3: **Spin dynamics under mw pumping.** (a) Bloch sphere with Zeeman frequencies renormalized due to exchange, $\omega_1 < \omega_Z < \omega_2$, and Rabi oscillations frequency, ω_R ; here $S_{t,\perp}^2 + S_{t,\parallel}^2 = \text{const}$ due to the spin conservation law. (b) Spin echo ($\pi/4 - \tau - 3\pi/4 - \tau$) with τ -dependent amplitude of echo signal due to difference of frequencies ω_1 and ω_2 .

out any electric circuits when noise is suppressed;

iii/ effective control of spin conversion between $S_{t,\perp}$ and $S_{t,\parallel}$ by microwave pulse takes place due to the interplay between exchange and Rabi oscillations;

iv/ formation of macroscopic spin patterns, with lateral sizes up to mm, using micromagnets in order to control REI-regime, see ¹⁸ and references therein;

v/ manipulation of single spins (or a few-spin clusters with exchange interaction) in ultra-pure Ge, with inter-donor distances $\geq 3 \mu\text{m}$ (concentrations $\leq 10^{11} \text{ cm}^{-3}$), ¹⁹ employing STM-technique, see²⁰ and references therein.

Results

Exchange via phonon modes. The spin subsystem of donors in Ge is described by the Hamiltonian $\hat{H}_s = (\hbar/2) \sum_k (\omega_Z \cdot \hat{\sigma}_k)$ with the Zeeman frequency $\omega_Z \parallel 0Z$ if magnetic field is perpendicular

to the Ge layer and $\hat{\sigma}_k$ is the Pauli matrix for k th donor placed at \mathbf{r}_k . Within the harmonic approach, the quantized acoustic modes is described by $\hat{H}_{ph} = \sum_{\nu\mathbf{q}} \hbar\omega_{\nu\mathbf{q}} \hat{b}_{\nu\mathbf{q}}^\dagger \hat{b}_{\nu\mathbf{q}}$ and the spin-lattice interaction is introduced in analogy to the bulk case,¹¹ taking into account modifications of the vibration spectra in PC or r/Ge/r structure (see details in Supplementary Note 1 and Supplementary Figs. 1-4):

$$\hat{H}_{sph} = \sum_{\nu\mathbf{q}} g_{\nu\mathbf{q}} \hat{\sigma}_k \cdot \xi_{\mathbf{r}_k}^{(\nu\mathbf{q})} \hat{b}_{\nu\mathbf{q}} + H.c. \quad (1)$$

Here $b_{\nu\mathbf{q}}^\dagger$ and $b_{\nu\mathbf{q}}$ are the creation and annihilation boson operators for mode of frequency $\omega_{\nu\mathbf{q}}$ with 2D wave vector \mathbf{q} (which varies over the first Brillouin zone in the case of PC, $|\mathbf{q}| < \pi/a$ for square lattice of period a) and ν labeled polarization and discrete quantum numbers. The components of vector $\xi_{\mathbf{r}_k}^{(\nu\mathbf{q})}$ are expressed through the strain tensor for donor at \mathbf{r}_k (averaging over the donor volume a_B provides the cut-off for wavelengths shorter the effective Borh radius^{12,13}, a_B , see Supplementary Note 2). The coupling constant $g_{\nu\mathbf{q}} = K\hbar\omega_Z\sqrt{\hbar/2\rho\omega_{\nu\mathbf{q}}V}$ is determined through the Ge density, ρ , the normalization volume, V , and the dimensionless factor $K \sim (1 \text{ or } 7.5) \times 10^3$ for As or Sb donors.

Within the second order accuracy with respect to \hat{H}_{sph} , we transform the total Hamiltonian into¹⁴

$$\hat{\mathcal{H}}_{eff} = \hat{H}_s + \hat{H}_{ph} + \left[\hat{H}_{sph}, \frac{i}{\hbar} \int_{-\infty}^0 dt e^{\lambda t} \hat{H}_{sph}(t) \right] \hat{H}_{sph}(t) = \sum_{\nu\mathbf{q}k\alpha} g_{\nu\mathbf{q}} \hat{\sigma}_{k\alpha}(t) \xi_{\mathbf{r}_k}^{(\nu\mathbf{q})} e^{i\mathbf{q} \cdot \mathbf{x}_k} \hat{b} e^{i\omega_{\nu\mathbf{q}} t} + H.c. , \quad (2)$$

where the circular components of spin are $\hat{\sigma}_{k\alpha}(t) = \hat{\sigma}_{k\alpha} \exp(i\alpha\omega_Z t)$ with $\alpha = \pm 1$ and the plane-wave factors $\exp(i\mathbf{q} \cdot \mathbf{x}_k)$ are separated. After averaging of $\hat{\mathcal{H}}_{eff}$ over the phonon thermostat

with the density matrix $\hat{\eta}_{ph}$ ($\text{Tr}_{ph} \dots$ is the trace over boson variables) we obtain the effective spin Hamiltonian for the donor spins, $\widehat{H}_{eff} = \text{Tr}_{ph} \hat{\eta}_{ph} (\widehat{\mathcal{H}}_{eff} - \widehat{H}_{ph})$, which takes into account the renormalization of Zeeman splitting (polaron effect) and the exchange interaction via phonons, \widehat{H}_{SS} .

The polaron contribution is added to \widehat{H}_s which contains now the renormalized Zeeman frequency $\omega_{Zk} = \omega_Z + \Delta\omega_k$. The ratio $\Delta\omega_k/\omega_Z$ is up to 2×10^{-4} for Sb donor and is weakly dependent on temperature and on donor position in unit cell of PC or across r/Ge/r-structure, see details in Supplementary Note 3. The exchange Hamiltonian is given by

$$\widehat{H}_{SS} = \sum_{\substack{\alpha\alpha'kk' \\ (k \neq k')}} J_{\alpha\alpha'}^{(kk')} \hat{\sigma}_{k\alpha} \hat{\sigma}_{k'\alpha'}, \quad (3)$$

where the exchange matrix $J_{\alpha\alpha'}^{(kk')}$ has a non-zero circular components only. This matrix is given by

$$J_{\alpha\alpha'}^{(kk')} = \sum_{\nu\mathbf{q}} \frac{g_{\nu\mathbf{q}}^2}{\hbar} \left(\frac{\xi_{\mathbf{r}_{k'}, -\alpha'}^{(\nu\mathbf{q})} \xi_{\mathbf{r}_k, \alpha}^{(\nu\mathbf{q})*}}{\omega_{\nu\mathbf{q}} + \alpha' \omega_Z} e^{-i\mathbf{q} \cdot \Delta\mathbf{x}_{kk'}} + \frac{\xi_{\mathbf{r}_k, -\alpha}^{(\nu\mathbf{q})} \xi_{\mathbf{r}_{k'}, \alpha'}^{(\nu\mathbf{q})*}}{\omega_{\nu\mathbf{q}} - \alpha' \omega_Z} e^{i\mathbf{q} \cdot \Delta\mathbf{x}_{kk'}} \right) \quad (4)$$

and there is a strong large-scale dependence on the inter-donor distance $\Delta\mathbf{x}_{kk'} = \mathbf{x}_k - \mathbf{x}_{k'}$, while dependencies of $\xi_{\mathbf{r}_k}^{(\nu\mathbf{q})}$ on \mathbf{r}_k are vanished under averaging over transverse coordinates $z_k, z_{k'}$ [here $\mathbf{r} = (\mathbf{x}, z)$] and over lateral donor positions in the unit cell of PC.

Donor-based qubit. We consider the averaged exchange integral $\langle \widehat{J}^{(kk')} \rangle$ replacing the exponential contribution $\langle \exp(i\mathbf{q} \cdot \Delta\mathbf{x}_{kk'}) \rangle$ by the zero order Bessel function $J_0(q\Delta x)$ where Δx is the mean inter-donor distance. After replacing $\xi_{\dots}^{(\nu\mathbf{q})} \xi_{\dots}^{(\nu\mathbf{q})*} / (\omega_{\nu\mathbf{q}}^2 - \omega_Z^2)$ as a_ν / \bar{c}^2 , where \bar{c} a character-

istic velocity and coefficients $a_\nu \sim 1$, the ratio of the exchange integral to the Zeeman energy is estimated as

$$\frac{J_{\Delta x}}{\hbar\omega_Z} \sim \frac{K^2\hbar\omega_Z}{4\pi\rho d\bar{c}^2} \sum_\nu a_\nu \int_0^{q_m} dq q J_0(q\Delta x) \sim \frac{K^2\hbar\omega_Z}{4\pi M_{\Delta x}\bar{c}^2} A_{\Delta x}, \quad q_m \sim \pi/a_B. \quad (5)$$

Here we introduce the factor $A_{\Delta x} = \sum_\nu a_\nu \int_0^{q_m} dq \dots$ and $M_{\Delta x} \approx \rho d \Delta x^2$ estimated mass of Ge vibrated between spins. Here $A_{\Delta x} \gg 1$ because the cut-off factor $\sqrt{\pi\Delta x/a_B}$ in $\int_0^{q_m} dq \dots$ and $J_{\Delta x}$ decreases slower Δx^{-2} . We perform numerical estimates of (5) for Sb donor assuming $d \simeq 100$ nm. Using $\omega_Z = 15$ GHz (if ω_Z is approaching to the gap edges, an additional resonant enhancement of $A_{\Delta x}$ takes place) and taking \bar{c} as an averaged sound velocity of Ge we obtain $J_{\Delta x}/\hbar\omega_Z \sim 3A_{\Delta x} \times 10^{-7}$ i.e $J_{\Delta x}/\hbar$ ranges up to $30 \div 90$ kHz if $\Delta x \sim d$.

This result should be modified under the REI-regime, when ω_Z approaches edge of gap, ω_G , and $\Delta x \geq d$, so that the near-edge mode gives a main contribution to $J_{\Delta x}$. For these conditions, $J_{\Delta x}/\hbar\omega_Z$ is transformed into

$$\frac{J_{\Delta x}}{\hbar\omega_Z} \sim \frac{K^2\hbar\omega_Z}{4\pi\rho d} \frac{|\xi_0|^2}{2\omega_Z^2} \int_0^{q_m} \frac{dq q J_0(q\Delta x)}{\delta_Z^2 + (q/q_1)^2} \sim \frac{K^2\hbar\omega_Z}{M_d(d\omega_Z)^2} K_0(\delta_Z q_1 \Delta x), \quad M_d = \rho \left(\frac{2d}{\pi} \right)^3, \quad (6)$$

where the energy $M_d(d\omega_Z)^2$ in the denominator is estimated with the use $|\xi_0| \sim \pi/d$ and parabolic dispersion of mode, $\omega_G[1 + (q/q_1)^2]$, written through $q_1 \sim \pi/d$. The argument of the modified Bessel function of second kind, $K_0(y)$, is determined by the relative detuning $\delta_Z = \sqrt{(\omega_G - \omega_Z)/\omega_Z}$ multiplied by Δx . The exponential suppression of $J_{\Delta x}$ for $\Delta x > d/\pi\delta_Z$ and slow (logarithmic) variations of $J_{\Delta x}$ if $d \leq \Delta x < d/\pi\delta_Z$ take place due to the asymptotics $K_0(y) \simeq \ln(2/y) - C$ or

$\sqrt{\pi/2y} \exp(-y)$ if $y > 1$ or $y \leq 1$; here C is the Euler's constant. For the parameters used, Eq. (6) gives $J_{\Delta x}/\hbar\omega_Z \sim 8.8K_0(\dots) \times 10^{-6}$ and $J_{\Delta x}/\hbar$ is in agreement with estimates for (5), if $\Delta x \sim d$.

In Fig. 4 we show the ratio $J_{\Delta x}/\hbar\omega_Z$ for the sandwiched r/Ge/r-structure versus inter-donor distance, which demonstrates a sharp suppression of the RIE-regime if δ_Z increases, see inset. If $\pi\delta_Z \geq 10^{-(3\div 4)}$ (disorder effects are discussed below), the REI-regime is realized over a wide interval of Δx , between 10 nm and 0.01÷0.1 cm. Similar dependencies of $J_{\Delta x}$ for PC with the dispersion relations of Fig. 1b show the REI-regimes if ω_Z approaches to the upper or lower edges of gap (M or Γ points of the Brillouin zone). The results for PC are more sensitive to lateral and transverse positions of donors in unit cell and, after averaging over donor distribution, $J_{\Delta x}$ differs from the above estimates by factor 0.5÷3. In general, the the exchange matrix in (3) can be modified using selective doping (lateral or across Ge layer) or orientation of magnetic field with respect to 0Z or to axis of PC.

Further, we turn to the longitudinal relaxation rate ν_1 in the structures under consideration. In PC at low ($\ll \hbar\omega_Z$) temperatures, ν_1 is determined by the two-phonon spin-flip transitions while in the r/Ge/r-structures ν_1 is caused by the spin-flip transitions via bulk phonons weakly penetrated into Ge layer, see Supplementary Note 4. We estimate the relative relaxation rate based on the golden rule with the forth-order ($\propto K^2$) matrix elements of in PC and accounting bulk modes,

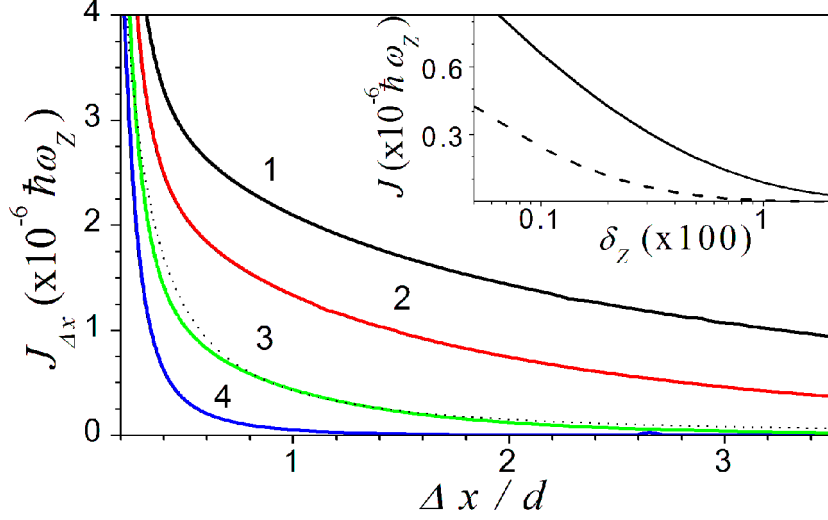


Figure 4: **Exchange integral.** $J_{\Delta x}$ versus Δx (in units $10^{-6}\hbar\omega_Z$ and d , respectively) for Ge layer sandwiched between rigid slabs under relative detunings δ_Z^2 : 10^{-3} (1), 5×10^{-3} (2), 0.05 (3), and 0.5 (4). Asymptotics $J_{\Delta x} \propto \Delta x^{-1.5}$ is shown by dotted curve and inset demonstrate \ln -dependency of $J_{\Delta x}/\hbar\omega_Z$ on δ_Z for $\pi\Delta x/d \simeq 5$ and 10 (solid and dashed curves, respectively).

weakly propagated through r/Ge/r-structure. The results are:

$$\frac{\nu_1}{\omega_Z} \sim \begin{cases} (K^2\hbar\omega_Z/M_I\tilde{c}^2)^2, & M_I = \rho d(\tilde{c}/\omega_Z)^2 \\ K^2\hbar\omega_Z/M_{II}\tilde{c}^2, & M_{II} = 2\pi\rho(\tilde{c}/\omega_Z)^3 \end{cases}. \quad (7)$$

Here the characteristic sound velocity \tilde{c} is combined from $c_{i,t}$ in Ge and rigid materials and $\nu_1 \propto \tilde{c}^5$ in r/Ge/r-structures. For the above parameters, we got $\nu_1/\omega_Z \leq 10^{-11}$ and ν_1^{-1} exceeds seconds. In PC $\nu_1 \propto \omega_Z^7$ and longitudinal relaxation time ν_1^{-1} exceeds hundreds seconds. Thus, $J_{\Delta x}/\hbar\nu_1$ exceeds 10^5 and in photonic gap ν_1 is negligible.

Bloch equation. Temporal evolution of weakly interacted spins randomly placed in PC or r/Ge/r-structure is described by the averaged spin vectors,¹⁵ $\mathbf{s}_{kt} = (1/2)\text{Tr}_S \hat{\boldsymbol{\sigma}}_k \hat{\rho}_t$, where $\hat{\rho}_t$ is the multi-spin density matrix governed by the equation with the Hamiltonian \hat{H}_{eff} . We restrict ourselves

by the second order accuracy on \widehat{H}_{SS} (the mean field approximation) and factorize the two-spin correlation function as $\text{Tr}_S \hat{\rho}_t \hat{\sigma}_{k,\alpha} \hat{\sigma}_{k',\beta} \approx s_{kt,\alpha} s_{k't,\beta}$, cf. Supplementary Note 5. As a result, the system of the nonlinear Bloch equations for \mathbf{s}_{kt} takes form:

$$\frac{d\mathbf{s}_{kt}}{dt} + \hat{\gamma} \cdot \mathbf{s}_{kt} = [(\boldsymbol{\omega}_{Zk} + \Delta\boldsymbol{\omega}_t) \times \mathbf{s}_{kt}] - \frac{2}{\hbar} \sum_{k' (k' \neq k)} \left[(\hat{J}^{(kk')} \cdot \mathbf{s}_{k't}) \times \mathbf{s}_{kt} \right]. \quad (8)$$

Here $\Delta\boldsymbol{\omega}_t$ is the time-dependent Zeeman frequency under a microwave pumping (below $\Delta\boldsymbol{\omega}_t \perp 0Z$), $\hat{\gamma} \cdot \mathbf{s}_{kt}$ describes relaxation of k th spin, and the last term is written through the effective exchange frequency with matrix (4). Under pumping $\Delta\boldsymbol{\omega}_{Zt}$ switched on at $t = 0$ Eq. (5) should be solved with the initial conditions $\mathbf{s}_{kt=0} = (0, 0, s_{k0})$ where $s_{k0} \simeq -1/2$ if temperature $\ll \hbar\omega_Z$ and $s_{k0} \rightarrow 0$ for high temperatures ($\gg \hbar\omega_{Zk}$).

Instead of a microscopic set $\{\mathbf{s}_{kt}\}$, we introduce the averaged spin orientation

$$\mathbf{S}_{\mathbf{x}t} = \left\langle \sum_k \delta(\mathbf{r} - \mathbf{r}_k) \mathbf{s}_{kt} \right\rangle / \left\langle \sum_k \delta(\mathbf{r} - \mathbf{r}_k) \right\rangle,$$

which is weakly dependent on transverse coordinate z . For the large ($\gg d, a$) scale inhomogeneity case $\mathbf{S}_{\mathbf{x}t}$ is governed by the spin diffusion equation

$$\begin{aligned} \frac{d\mathbf{S}_{\mathbf{x}t}}{dt} + \hat{\gamma} \cdot \mathbf{S}_{\mathbf{x}t} &= [\boldsymbol{\Omega}_{\mathbf{x}t} \times \mathbf{S}_{\mathbf{x}t}] - D [(\Delta_{\mathbf{x}} \mathbf{S}_{\mathbf{x}t,\perp}) \times \mathbf{S}_{\mathbf{x}t}], \\ \boldsymbol{\Omega}_{\mathbf{x}t} &\equiv \boldsymbol{\omega}_{Z\mathbf{x}} - \tilde{\omega}_{\mathbf{x}} \mathbf{S}_{\mathbf{x}t,\perp} + \Delta\boldsymbol{\omega}_t, \end{aligned} \quad (9)$$

where $\boldsymbol{\omega}_{Z\mathbf{x}}$ takes into account the non-uniform Lamb renormalization of ω_Z and the exchange

contribution is transformed into $-\tilde{\omega}_{\mathbf{x}} \mathbf{S}_{\mathbf{x}t,\perp}$, where $\mathbf{S}_{\mathbf{x}t,\perp}$ is the transverse part of spin orientation. The frequency $\tilde{\omega}_{\mathbf{x}}$ is determined by the averaged exchange integral $\langle \hat{J}^{(kk')}/\hbar \rangle$ with the non-zero and equal xx - and yy -components. The diffusion coefficient, D , is estimated as $\tilde{\omega} l_{ex}^2/2$ where l_{ex} estimates a scale of exchange interaction. The last contribution of (8) is negligible for the case of large-scale ($\gg l_{ex}$) inhomogeneities of $\omega_{Z\mathbf{x}}$ and $\tilde{\omega}_{\mathbf{x}}$. Because the ratio $\hbar\nu_1/J_{\Delta x}$ is negligible, we replace $\hat{\gamma} \cdot \mathbf{S}_{\mathbf{x}t}$ by $\nu_2 \mathbf{S}_{\mathbf{x}t,\perp}$ with the transverse relaxation rate ν_2 .

Taking into account ν_2 and neglecting diffusion if scale of disorder $> l_{ex}$, one obtains the nonlinear (with respect to $\mathbf{S}_{\mathbf{x}t}$ and $\Delta\omega_t$) system for the transverse and longitudinal ($\mathbf{e}_z S_{\mathbf{x}t,\parallel}$) parts of spin orientation

$$\begin{aligned} \left(\frac{d}{dt} + \nu_2 \right) \mathbf{S}_{\mathbf{x}t,\perp} &= \Omega_{\mathbf{x}t,\parallel} [\mathbf{e}_z \times \mathbf{S}_{\mathbf{x}t,\perp}] - \Delta\omega_t S_{\mathbf{x}t,\parallel} , \\ \frac{d}{dt} S_{\mathbf{x}t,\parallel} &= (\Delta\omega_t \cdot \mathbf{S}_{\mathbf{x}t,\perp}) . \end{aligned} \quad (10)$$

Here $\Omega_{\mathbf{x}t,\parallel} = \omega_{Z\mathbf{x}} + \tilde{\omega}_{\mathbf{x}} S_{\mathbf{x}t,\parallel}$ includes the Lamb shift and the exchange ($\propto S_{\mathbf{x}t,\parallel}$) renormalization. Within the collisionless regime, $\nu_2 t \ll 1$, the spin conservation takes place $S_{\mathbf{x}t,\perp}^2 + S_{\mathbf{x}t,\parallel}^2 = S_0^2$ with the $\mathbf{x}t$ -independent initial orientation S_0 . If $\Delta\omega_t \rightarrow 0$ and $\nu_2 \rightarrow 0$, Eq. (10) describes free rotation of $S_{\mathbf{x}t,\perp}$ around $0Z$ with the frequency $\omega_{Z\mathbf{x}} + \tilde{\omega}_{\mathbf{x}} S_0$. Characterization of PC and r/Ge/r-structure (exchange, relaxation, and disorder parameters) and manipulation of spins are possible under resonant microwave pumping.

Microwave response. The absorbed power is given by $P_{xt} = -\hbar \overline{\Delta \omega_t \cdot d\mathbf{S}_{xt,\perp}/dt}$, where (\dots) means averaging over period $2\pi/\omega$.^{10,16} Under weak circular pumping $\Delta \omega_{t,x} + i\Delta \omega_{t,y} = \omega_P \exp(i\omega t)$, the solution of linear Eq. (10) gives the resonant peak $P_x = \hbar \omega \omega_P^2 \nu_2 / [\nu_2^2 + (\delta \omega_x - \tilde{\omega}_x/2)^2]$ where $\delta \omega_x \equiv \omega - \omega_{Zx}$ is the frequency detuning and $S_0 = -1/2$ for zero-temperature limit. The resonant line has linewidth determined by ν_2 and by disordered contributions stem from $\delta \omega_x$ and $\tilde{\omega}_x$. If line is narrow enough, these contributions can be verified from the shape of dP/dH averaged over disorder, similarly to the measurements of GeSi dots.¹⁷ The derivative dP/dH increases under the REI-conditions due to additional dependency of $\tilde{\omega}$ on δ_Z .

In the case of weak exchange, $\tilde{\omega} \ll \max(\omega_P, |\delta \omega|, \nu_{1,2})$, the linear ($\propto S_0$) system (10) describes evolution of the resonant absorption P_{xt} and the spin orientation $S_{xt,\parallel}$. Neglecting damping, at $\nu_2 t \ll 1$ and $\nu_2 \ll \omega_P, |\delta \omega_x|$, and using the rotation wave approach, if $|\delta \omega| \ll \omega_Z$, one obtains oscillating responses

$$P_{xt} = -S_0 \hbar \omega \frac{\omega_P^2}{\omega_{xR}} \sin \omega_{xR} t, \quad S_{xt,\parallel} = S_0 \cos \omega_{xR} t \quad (11)$$

with the Rabi frequency $\omega_{xR} = \sqrt{\omega_P^2 + \delta \omega_x^2}$ and the $\pi/2$ phase shift between P_{xt} and $S_{xt,\parallel}$. If the exchange interaction is essential ($\tilde{\omega} \sim \omega_P, |\delta \omega|$), shape and strength of temporal Rabi oscillations are sensitive on $\tilde{\omega}/\omega_P$. Within the rotating-wave approximation, we plot these responses in Fig. 5 for low temperatures, $S_0 = -1/2$ at resonant condition $\delta \omega = 0$ (implicit solution for $S_{xt,\parallel}$ can be written through the elliptic integrals, see details in Supplementary Note 6). Shapes of temporal Rabi oscillations of P_t and $S_{t,\parallel}$ are modified with a suppression of their amplitudes and doubling of

periods around $\tilde{\omega}/\omega_P \sim 5.5$ due to an effective interplay between exchange and Rabi oscillations. Detuning ($\delta\omega \neq 0$) results in a shift of similar behavior to $\tilde{\omega}/\omega_P \sim 8$. The collisionless response is suppressed by decoherentization if $\nu_2 t \geq 1$, so that an effective manipulation of \mathbf{S}_t is possible with the use of pulse duration $t_p < \nu_2^{-1}$. More sharp peculiarities take place for the differential nonlinear absorption dP_t/dH .

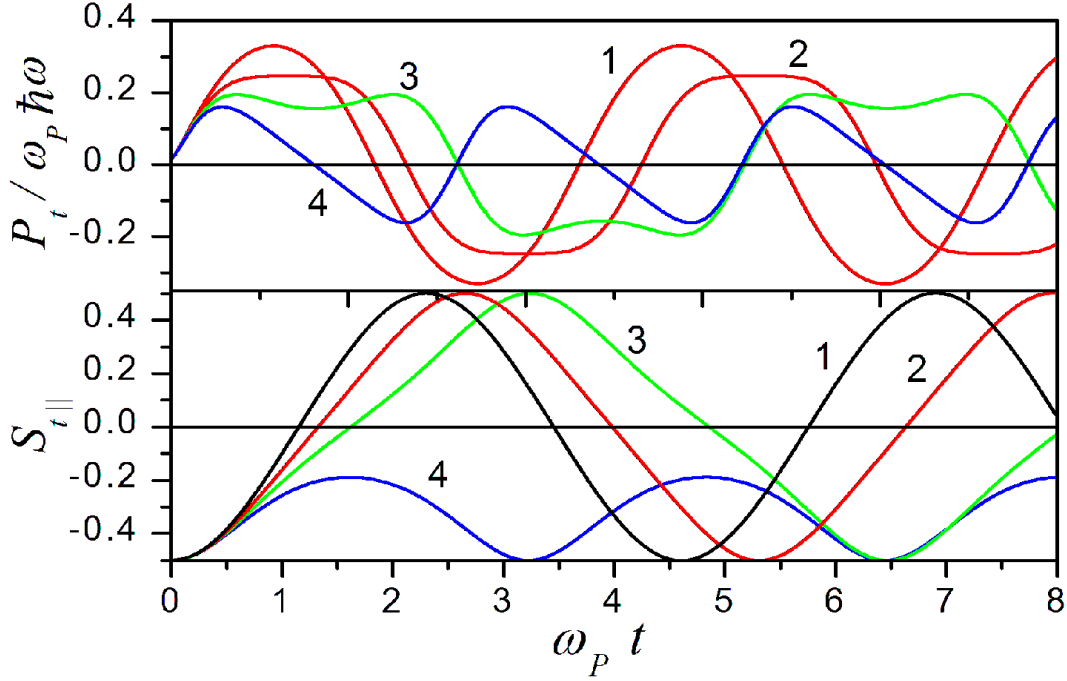


Figure 5: **Interplay between exchange and Rabi oscillations.** Absorbed power P_t (in units $\omega_P \hbar \omega$) and the longitudinal spin orientation $S_{t,\parallel}$ versus dimensionless time, $\omega_P t$, for $\Omega/\omega_P = 2$ (1), 4 (2), 5 (3), 6 (4).

The two-pulse spin echo scheme ($\pi/4 - \tau - 3\pi/4 - \tau \rightarrow \text{echo}$) permits verification of exchange contribution under an essential decoherentization and long-range disorder.¹⁰ Here the delay times $\tau \gg t_{1,2}$ and pulses of frequency ω and durations $t_{1,2}$ are connected with pumping levels $\omega_{P1,2}$ by $\omega_{P1} t_1 = \pi/4$ and $\omega_{P2} t_2 = 3\pi/4$. In the rotating-wave frame, free evolution of $\mathcal{S}_{t,\perp} = \langle S_{t,x} + iS_{t,y} \rangle \exp(-i\omega t)$ after first and second pulses is $\propto \exp(\delta\omega_{1,2} t)$ with different

frequencies $\delta\omega_{1,2} = \delta\omega_{\mathbf{x}} - \tilde{\omega}S_{1,2\parallel}$ and $\langle \dots \rangle$ stands for averaging over long-range disorder. If $\omega_{P1,2} \gg \tilde{\omega}, |\delta\omega_{\mathbf{x}}|, \nu_2$ and exchange is negligible according to Fig. 5, the spin orientations after first and second pulses are $S_{1,\parallel} = S_0/\sqrt{2}$ [c.f. Eq. (11)] and $S_{2,\parallel} = -S_0(1 + \cos \delta\omega_1\tau)/2$. For the case of Gaussian disorder with the averaged variations of Zeeman frequency $\sqrt{\langle \delta\omega_{\mathbf{x}}^2 \rangle} = \delta\omega^*$, spin echo signal is

$$\mathcal{S}_{t,\perp} = \bar{S}_0 \exp \left\{ -\frac{[\delta\omega^*(t - 2\tau)]^2}{2} \right\} \Psi(\phi_\tau), \quad (12)$$

where $\bar{S}_0 = (1 + \sqrt{2})/4$ stands for the echo amplitude at $t = 2\tau$ if $\tilde{\omega} \rightarrow 0$ and $\Psi(0) = 1$. Function $\Psi(\phi_\tau)$ with $\phi_\tau = S_0\tilde{\omega}\tau/\sqrt{2}$ describes modulation of $\mathcal{S}_{t,\perp}$ caused by the exchange-induced difference in $\delta\omega_1$ and $\delta\omega_2$, which results in an interference oscillations of $\Psi(\phi_\tau)$. The disorder-induced exponent and the modulation Ψ are multiplied because of additive contributions of these factors to the frequency $\Omega_{\mathbf{x}t,\parallel}$ in Eq. (10). Shape of modulation of $\mathcal{S}_{t=2\tau,\perp}$ versus delay time τ is determined by $\text{Re}\Psi$ and $\text{Im}\Psi$ plotted in Fig. 6. Here $\text{Re}\Psi$ and $\text{Im}\Psi$ are even and odd functions of ϕ_τ and $\phi_\tau > 0$ corresponds to the spin inversion case, $S_0 > 0$. Thus, verification of exchange contribution require variations of τ in $\sim 10 \mu\text{s}$ scales.

Discussion

It is important to stress that these results are based on the estimates written through the ratios of $K^2\hbar\omega_Z$ to the characteristic energies (factors $M_{\dots}c^2$ in denominators), which are evident from the dimensional requirements. The evaluation of \widehat{H}_{SS} is restricted by donor concentrations $n_D \ll 10^{16} \text{ cm}^{-3}$, when the exchange due to tunneling overlap of donors is negligible. For lower concentra-

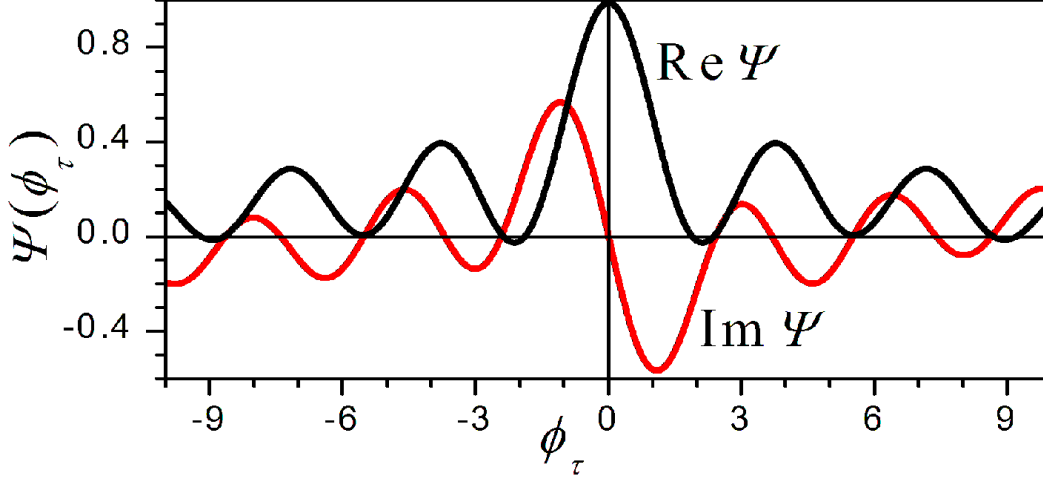


Figure 6: **Oscillations of spin echo amplitude.** Real and imaginary parts of Ψ versus delay time τ and S_0 (here $\phi_\tau = S_0 \tilde{\omega} \tau / \sqrt{2}$).

tions, the mean-field approximation for exchange in Eqs. (8-10) is valid if $n_D^{-1/3} < \text{radius of interaction}$. A region of intermediate concentrations, between the mean-field regime and a system of free donor spins (if $n_D \leq 10^{11} \text{ cm}^{-3}$) requires a special analysis.

In order to implement the structures suggested and to measure the peculiarities found, ?? one have to meet several technological requirements for PC or r/Ge/r-structures: **a)** suppression of spin decoherencization rate ν_2 in comparison to typical values in Ge-based materials^{7,21} **b)** reduced stresses, dislocations, and interface disorder, **c)** homogeneity of donor distribution in PC or r/Ge/r-structures or possibility for selective doping,^{22?} far from imperfections at boundaries or interfaces, and **d)** spatio-temporal stability of magnetic field and pumping characteristics, i.e. ω_Z , ω , and ω_P , as well as frequency of gap edge allowed realization of REI-regime.

To conclude, we have demonstrated that a combination of phonon engineering provided gap in vibration spectra in PC or r/Ge/r-structure with unique spin and technological characteristics of

Ge opens a way for quantum information applications. We believe that our paper will stimulate effort for preparation of structures suggested and for verification of qbit parameters.

Methods

Theoretical background. Spin-lattice interaction in structures with phononic gap is considered by the classical procedure^{11,12}, based on the elastodynamics of continuous media.²³ The Bloch equation for averaged spin density is evaluated within the mean-field approach, which corresponds to the long-range exchange interaction. The nonlinear spin dynamics is examined with the simplified description of decoherentization through ν_2 for the long-range inhomogeneities case.

Numerical simulation. The eigenmodes and eigenstates for the elastic vibration problem in PC or in r/Ge/r-structure are analyzed with the use of the finite elements method realized via Comsol Multiphysics software. The PC was designed as the structural mechanic modulus (unit cells) connected via the in-plane periodic (Bloch-Floquet) boundary conditions. The free boundary conditions are applied at all other surfaces. Standard numerical methods have been used for simulation of the exchange interaction and the nonlinear spin dynamics (the interplay of Rabi oscillations and exchange, or the spin echo modulation). More details of our calculations can be found in Supplementary Materials.

References

1. Ladd, T. D., Jelezko, F., Laflamme, R., Nakamura, Y., Monroe, C. & O'Brien, J. L. Quantum comput-

- ers. *Nature* **464**, 45-53 (2010).
2. Kloeffer, C. & Loss, D. Prospects for Spin-Based Quantum Computing in Quantum Dots. *Annu. Rev. Condens. Matter Phys.* **4**, 51-81 (2013).
 3. Kane, B. E. A silicon-based nuclear spin quantum computer. *Nature* **393**, 133-137 (1998).
 4. Dutt, M. V. G., Childress, L., Jiang, L., Togan, E., Maze, J., Jelezko, F., Zibrov, A. S., Hemmer, P. R. & Lukin, M. D. Quantum Register Based on Individual Electronic and Nuclear Spin Qubits in Diamond. *Science* **316**, 1312-1316 (2007).
 5. Smelyanskiy, V.N., Petukhov, A. G. & Osipov, V.V. Quantum computing on long-lived donor states of Li in Si. *Phys. Rev. B* **72**, 081304 (2005). ADD ??
 6. Tyryshkin, A. M., Tojo, S., Morton, J. J. L., Riemann, H., Abrosimov, N. V., Becker, P., Pohl, H.-J., Schenkel, T., Thewalt, M. L. W., Itoh, K. M. & Lyon, S. A. Electron spin coherence exceeding seconds in high-purity silicon. *Nature Materials* **11**, 143 (2012).
 7. Claeys, C. & Simoen, E. *Germanium-based technologies: from materials to devices* (Elsevier, Amsterdam,, 2011).
 8. Safavi-Naeini, A. H., Mayer Alegre, T. P., Chan, J., Eichenfield, M., Winger, M., Lin, Q., Hill, J. T., Chang, D. E. & Painter, O. Electromagnetically induced transparency and slow light with optomechanics. *Nature* **472**, 69 (2011).
 9. *Handbook Series on Semiconductor Parameters*, v. 1, Eds. Levinshtein, M., Rumyantsev, S., & Shur, M. (World Scientific, 1996).
 10. Schweiger A. & Jeschke, G. *Principles of Pulse Electron Paramagnetic Resonance* (Oxford University Press, Oxford, 2001).

11. Roth, L. *g* Factor and Donor Spin-Lattice Relaxation for Electrons in Germanium and Silicon. *Phys. Rev.* **118** 1534-1540 (1960).
12. Hasegawa, H., Spin-Lattice Relaxation of Shallow Donor States in Ge and Si through a Direct Phonon Process. *Phys. Rev.* **118**, 1523-1534 (1960).
13. Solenov, D., Tolkunov, D. & Privman, V. Exchange interaction, entanglement, and quantum noise due to a thermal bosonic field. *Phys. Rev. B* **75** 035134 (2007).
14. Kittel, C. *Quantum Theory of Solids*, (John Wiley, New York, 1987).
15. *Spin Physics in Semiconductors*, Ed. Dyakonov, M.I. (Springer, Berlin/Heidelberg, 2008).
16. *Electron Spin Resonance and Related Phenomena in Low-Dimensional Structures*, Ed. Fanciulli, M. (Springer, Berlin 2009).
17. Zinovieva, A. F., Stepina, N. P., Nikiforov, A. I., Nenashev, A. V., Dvurechenskii, A. V., Kulik, L. V., Carmo, M. C. & Sobolev, N. A. Spin relaxation in inhomogeneous quantum dot arrays studied by electron spin resonance. *Phys. Rev. B* **89**, 045305 (2014).
18. Pioro-Ladriere, M., Obata, T., Tokura, Y., Shin, Y.-S., Kubo, T., Yoshida, K., Taniyama, T. & Tarucha S. Electrically driven single-electron spin resonance in a slanting Zeeman field. *Nature Physics* **4**, 776 - 779 (2008)
19. Haller, E.E., Hansen, W.L. & Goulding, F.S. Physics of ultra-pure germanium *Adv. in Phys.* **30**, 93-138 (1981).
20. Durkan, C. & Welland, M. E. Electronic spin detection in molecules using scanning-tunneling-microscopy-assisted electron-spin resonance. *Appl. Phys. Lett.* **80**, 458 (2002). ???

21. Vrijen, R., Yablonovitch, E., Wang, K., Jiang, H. W., Balandin, A., Roychowdhury, V., Mor, T. & DiVincenzo, D. Electron-spin-resonance transistors for quantum computing in silicon-germanium heterostructures. *Phys. Rev. A*, **62**, 012306 (2000). ??
22. ?? selective doping (lateral or across Ge layer) ??
23. Strosio, M. A., & Dutta, M. *Phonons in Nanostructures*. (Cambridge Univ. Press, 2001).

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Author Contributions F.W. performed the calculations. All authors analysed and discussed the results. F.W and E.M. wrote the paper with major input from A.K. ??

Additional Information

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